chain nodes :

7 8 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 chain bonds:

4-8 5-46 6-7 9-40 10-34 11-39 14-41 17-37 18-36 19-35 20-38 22-45 24-42 25-43 26-44 29-47 30-48 31-33 32-49 ring bonds:

ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 2-16 \quad 2-13 \quad 2-21 \quad 2-27 \quad 3-4 \quad 4-5 \quad 5-6 \quad 9-10 \quad 9-14 \quad 10-11 \quad 11-12$

1-2 1-6 2-3 2-16 2-13 2-21 2-27 3-4 4-5 5-6 12-15 23-28 exact bonds:

4-8 5-46 6-7 9-40 10-34 11-39 14-41 17-37 18-36 19-35 20-38 22-45 24-42 25-43 26-44 29-47 30-48 31-33 32-49 normalized bonds:

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 18:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 40:CLASS 40:CLASS 42:CLASS 43:CLASS 44:CLASS 43:CLASS 44:CLASS 45:CLASS 47:CLASS 48:CLASS 49:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS

L1 STRUCTURE UPLOADED

=> d his

(FILE 'HOME' ENTERED AT 18:08:22 ON 17 SEP 2008)

FILE 'REGISTRY' ENTERED AT 18:08:41 ON 17 SEP 2008

Structure attributes must be viewed using STN Express query preparation.

=> s 11 SAMPLE SEARCH INITIATED 18:13:32 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 0 TO PROJECTED ANSWERS: 0 TO

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 18:13:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

 COST IN U.S. DOLLARS
 SINCE FILE ENTRY SESSION FULL ESTIMATED COST
 TOTAL SHIPTY SESSION FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 18:14:02 ON 17 SEP 2008